

Quantum Simulation of Molecular Collisions with Superconducting Qubits

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We introduce a protocol for the fast simulation of n -dimensional quantum systems on n -qubit quantum computers with tunable couplings. A mapping is given between the control parameters of the quantum computer and the matrix elements of $H_s(t)$, an arbitrary, real, time-dependent $n \times n$ dimensional Hamiltonian that is simulated in the n -dimensional ‘single excitation’ subspace of the quantum computer. A time-dependent energy/time rescaling minimizes the simulation time on hardware having a fixed coherence time. We demonstrate how three tunably coupled phase qubits simulate a three-channel molecular collision using this protocol, then study the simulation’s fidelity as a function of total simulation time.

A quantum computer can significantly reduce the resources necessary to simulate quantum mechanical systems [1]. Typically, quantum simulation algorithms construct the simulated system’s time evolution operator, energies and/or eigenstates from a universal set of gates [2–8]. Alternatively, ultracold atoms, trapped ions, and liquid-state NMR have directly emulated the time evolution of certain other quantum systems [9–11]. Recent experimental progress suggests that quantum simulation will be one of the first practical applications of quantum computation [7–12].

In principle, an n -qubit quantum computer can store the state of any $N = 2^n$ dimensional quantum system, an exponential reduction in the resources necessary to store quantum information on a classical computer. However, simulation may require $\sim N^2 = 2^{2n}$ elementary gates per time step unless the simulated Hamiltonian has special properties, e.g. locality [2, 13]. Even for these special Hamiltonians, fully digital quantum simulation often requires an excessive number of gates for current quantum computing technology [4, 6].

In this Letter, we show that a subspace of a tunable n -qubit quantum computer can emulate an arbitrary n -dimensional quantum system, trading an exponential reduction in resources for simulations of a wider variety of Hamiltonians. This subspace simulates other quantum systems very different from the computer itself in an amount of time that is independent of n . By comparison, classical simulation of an n -dimensional quantum system requires $\sim n^3$ elementary operations per time step. While the most efficient quantum simulation algorithms offer an exponential reduction in both qubits and elementary operations, they typically apply to specific, fundamental time-independent Hamiltonians, or those already similar to that of the computer itself. We show that with a more modest polynomial reduction in resources, a subspace of a tunable quantum computer can simulate any real, time-dependent Hamiltonian.

We begin by outlining the theory behind our approach to simulation. First, we identify an n -dimensional invariant subspace suitable for quantum simulation. Then we define a time dependent energy/time rescaling that maximizes the speed of the simulation within the constraints of the quantum computer. Finally, the control parameters of the quantum computer are given explicitly as a function of the matrix elements of $H_s(t)$.

Our approach is tested by performing a simulation of a molecular collision with a circuit of tunably coupled Josephson phase qubits. Molecular collisions and electronic structure calculations are widely studied as important applications of quantum simulation techniques [6–8]. We show in detail how a superconducting circuit of three tunably coupled Josephson phase qubits simulates a three channel Na-He collision. Finally, we discuss the relationship between simulation fidelity and total simulation time for this particular example.

An *n -Dimensional Subspace* of the full quantum computer’s Hilbert space, \mathcal{H} , can emulate another quantum system at all times only if it is invariant to the time evolution generated by the computer’s Hamiltonian H_{qc} (so that the subspace is well-isolated from the rest of \mathcal{H} and evolves unitarily). We model H_{qc} as

$$H_{qc}(t) = \sum_{i=1}^n -\frac{\epsilon_i(t)}{2} \sigma_i^z + \frac{1}{2} \sum_{i \neq j} g_{ij}(t) J_{\mu\nu} \sigma_i^\mu \otimes \sigma_j^\nu, \quad (1)$$

where $\epsilon_i(t)$ are the uncoupled qubit energies, $g_{ij}(t) = g_{ji}(t)$ are the pairwise qubit interaction strengths, $J_{\mu\nu}$ gives the relative size of the $\sigma_i^\mu \otimes \sigma_j^\nu$ interaction, and $\mu, \nu \in \{0, x, y, z\}$ are summed over. While $\epsilon_i(t)$ and $g_{ij}(t)$ may in general be time-dependent, the time-independent structure of qubit interaction is specified by $J_{\mu\nu}$, a dimensionless tensor that is typically fixed by a given architecture and is identical between each pair of qubits. In the weak coupling limit, $|g_{ij}| |J_{\mu\nu}| / \epsilon_i \ll 1$, subspaces of \mathcal{H} are invariant to time evolution generated by H_{qc} if

spanned by computational basis states having the same number of excited (tunable) qubits. The ‘single excitation subspace’, denoted as \mathcal{H}_n , is an n -dimensional invariant subspace spanned by $|i\rangle_n \equiv |00\dots 01_i\dots 0_n\rangle$ for all $i = 1, 2, \dots, n$.

The control parameters $\epsilon_i(t)$ and $g_{ij}(t)$ directly control the Hamiltonian that \mathcal{H}_n simulates. We define H_n as H_{qc} projected into the single excitation subspace,

$$H_n(t) \equiv PH_{qc}(t)P^\dagger \quad (2)$$

where P is an $n \times 2^n$ dimensional operator that projects \mathcal{H} onto \mathcal{H}_n . Up to an additive energy shift, H_n has matrix elements

$$H_n^{ij}(t) \equiv \begin{cases} \epsilon_i(t) - \alpha \sum_{k \neq i} g_{ik}(t), & i = j \\ g_{ij}(t), & i \neq j \end{cases} \quad (3)$$

with $\alpha \equiv 2(J_{zo} + J_{zz})$. We assume $J_{xx} + J_{yy} \neq 0$ and normalize $J_{\mu\nu}$ so that $J_{xx} + J_{yy} = 1$. In the weak coupling limit, \mathcal{H}_n is approximately invariant and generated by H_n :

$$\begin{aligned} U_n(t) &\equiv PU_{qc}(t)P^\dagger \\ &\simeq \mathcal{T}e^{-\frac{i}{\hbar} \int_0^t H_n(t')dt'} \end{aligned} \quad (4)$$

where \mathcal{T} is the time-ordering operator. H_n generates U_n exactly when no matrix elements of H_{qc} mix \mathcal{H}_n with the rest of \mathcal{H} (i.e. $J_{0x} = J_{0y} = J_{zx} = J_{zy} = 0$). The $(n^2 + n)/2$ parameters $\epsilon_i(t)$ and $g_{ij}(t)$ independently control each of the $(n^2 + n)/2$ matrix elements of the real H_n and can therefore be used to simulate any arbitrary, real Hamiltonian in \mathcal{H}_n .

While we can simulate H_s in \mathcal{H}_n by choosing $\epsilon_i(t)$ and $g_{ij}(t)$ so that $H_n(t) = H_s(t)$ for all t , a direct mapping between Hamiltonians limits the computer to simulating other quantum systems with similar energy scales over lengths of time within the computer’s coherence time. Fortunately, simulation of H_s only requires equality up to an overall phase between U_n and the time evolution operator generated by H_s :

$$\begin{aligned} U(t) &\equiv \mathcal{T}e^{-\frac{i}{\hbar} \int_{t_i}^t H_s(t')dt'} \\ &= e^{i\phi(t)} U_n(t_{qc}(t)). \end{aligned} \quad (5)$$

The time elapsed on the quantum computer, $t_{qc}(t)$, is a strictly increasing function of simulated time t , admitting a much less restrictive relationship between Hamiltonians:

$$H_s(t) + c(t) = \lambda(t)H_n(t_{qc}(t)). \quad (6)$$

$c(t)$ is a time-dependent, additive energy shift giving the overall phase difference $\phi(t) = \frac{1}{\hbar} \int_{t_i}^t c(t')dt'$, and we have introduced a positive, time-dependent energy/time scaling

$$\lambda(t) \equiv dt_{qc}/dt. \quad (7)$$

The energy/time scaling $\lambda(t)$ determines the speed of the simulation. By carefully minimizing $\lambda(t)$, we reduce the total simulation time and, consequently, the error due to decoherence. $\lambda(t)$ is bounded from below by experimental constraints on the allowed values of control parameters $\epsilon_i(t)$ and $g_{ij}(t)$ as well as their maximum rates of change. Suppose qubit interaction strengths can vary in a range $g_{ij}(t) \in [-g_{\max}, g_{\max}]$, and the uncoupled qubit energies can vary in a range $\epsilon_i(t) \in [\epsilon_{\min}, \epsilon_{\max}]$. For convenience, we define a simulated energy $E_i(t)$ analogous to $\epsilon_i(t)$ when diagonal contributions from qubit interactions are anticipated:

$$E_i(t) \equiv H_s^{ii}(t) + \alpha \sum_{j \neq i} H_s^{ij}(t). \quad (8)$$

Using this definition together with equations (3) and (6), we relate the control parameters of the quantum computer to the simulated energies in $H_s(t)$:

$$\begin{aligned} g_{ij}(t) &= H_s^{ij}(t)/\lambda(t) \\ \epsilon_i(t) &= [E_i(t) - c(t)]/\lambda(t). \end{aligned} \quad (9)$$

By choosing $c(t) = E_{\max}(t) - \lambda(t)\epsilon_{\max}$ where $E_{\max}(t)$ is the largest value obtained by the $E_j(t)$ at a particular t , we force each ϵ_i to be as large as possible and therefore minimize leakage out of \mathcal{H}_n .

Each of the computer’s control parameters remains within its allowed range when $\lambda(t)$ is larger than $(n^2 + n)/2$ energy ratios at all times:

$$\lambda(t) \geq \begin{cases} |H_s^{ij}(t)|/g_{\max}, & i \neq j \\ \Delta E_i(t)/\Delta \epsilon_{\max} \end{cases} \quad (10)$$

where $\Delta E_i(t) \equiv E_{\max}(t) - E_i(t)$ and $\Delta \epsilon \equiv \epsilon_{\max} - \epsilon_{\min}$. $\lambda(t)$ is also bounded by constraints on the speeds with which control parameters can change. Suppose $v_i^\epsilon(t_{qc}) \equiv d\epsilon_i(t_{qc})/dt_{qc}$ and $v_{ij}^g(t_{qc}) \equiv dg_{ij}(t_{qc})/dt_{qc}$ can never be larger in magnitude than v_{\max}^ϵ and v_{\max}^g respectively. Then for all t ,

$$v_{\max}^g \geq \frac{1}{\lambda^2} \left| \frac{dH_s^{ij}(t)}{dt} - \frac{H_s^{ij}(t)}{\lambda} \frac{d\lambda}{dt} \right| \quad (11)$$

(and similarly for v_{\max}^ϵ).

To simulate $H_s(t)$ in \mathcal{H}_n , we first choose $\lambda(t)$ as small as both inequalities (10) and (11) allow, guaranteeing a fast simulation within the experimental constraints of the quantum computer. We integrate over $\lambda(t)$ to calculate t_{qc} as a function of t :

$$t_{qc}(t) = \int_{t_i}^t \lambda(t')dt' + t_{qc}(t_i). \quad (12)$$

With both $\lambda(t)$ and $t_{qc}(t)$ known, we can explicitly map the matrix elements of H_s to the control parameters of the quantum computer:

$$\begin{aligned} \epsilon_i(t_{qc}(t)) &= \epsilon_{\max} + \Delta E_i(t)/\lambda(t) \\ g_{ij}(t_{qc}(t)) &= H_s^{ij}(t)/\lambda(t). \end{aligned} \quad (13)$$

To demonstrate our theory in detail, we describe three Josephson phase qubits simulating a three-channel collision between a sodium and a helium atom. For three phase qubits with tunable inductive coupling,

$$H_{\text{qc}}(t) = \sum_{i=1}^3 -\frac{\epsilon_i(t)}{2} \sigma_i^z + \frac{1}{2} \sum_{i \neq j} g_{ij}(t) \hat{\Phi}_i \otimes \hat{\Phi}_j \quad (14)$$

where $\hat{\Phi}_i$ is defined in terms of the matrix elements $\varphi_{jk} = \langle j | \hat{\varphi}_i | k \rangle$ of the local Josephson phase operator in the computational basis of the i th qubit:

$$\hat{\Phi}_i \equiv \sigma_i^x + \frac{\varphi_{00} - \varphi_{11}}{2\varphi_{01}} \sigma_i^z + \frac{\varphi_{11} + \varphi_{00}}{2\varphi_{01}} \sigma_i^0. \quad (15)$$

Both the ϵ_i and the φ_{jk} depend on Φ_x , the externally applied flux through the superconducting circuit. External flux bias is quantified by a dimensionless parameter $s_i(t) = \Phi_x / \Phi_x^*$ where Φ_x^* is the qubit's critical flux bias, or alternatively, by the dimensionless well depth $\Delta U / \hbar \omega_p$ [14]. We consider external bias values for which $s \in [.89, .90]$ and $\Delta U / \hbar \omega_p \in [13.7, 15.5]$. In this range, $\Delta \epsilon / h = 190 \text{ MHz}$ while $\hat{\Phi}_i \simeq \sigma_i^1 + 11\sigma_i^0$ varies little. A tunable mutual inductance independently controls the couplings $g_{ij}(t)$ between each pair of qubits. We have assumed Josephson junction parameters $I_0 = 2.93 \mu\text{A}$, $C = 1.52 \text{ pF}$, and $L = 808 \text{ pH}$.

An n -dimensional subspace can simulate a molecular collision only after we project the full, many-body Hamiltonian of the interacting electrons and nuclei into an n -dimensional basis. We construct the collision Hamiltonian from Born-Oppenheimer energies and nonadiabatic couplings calculated previously for three molecular channels: $\text{Na}(3s) + \text{He}(1s^2)$ [$1^2\Sigma^+$] and $\text{Na}(3p) + \text{He}(1s^2)$ [$1^2\Pi$; $2^2\Sigma^+$] [15], labeled as $|1\rangle_s$, $|2\rangle_s$ and $|3\rangle_s$ respectively. The energies are stored for fixed values of the internuclear distance R , which we assume takes straight-line trajectories in a standard semiclassical approximation: $R(t) = \sqrt{b^2 + v^2 t^2}$ where v is the incoming particle's velocity and b is the impact parameter of the collision.

Figure 1 outlines our simulation protocol for $H_s(t)$ describing a three-channel Na-He collision. The matrix elements of $H_s(t)$ are displayed in Fig. 1(a) for a given semiclassical trajectory $R(t)$. Directly below, we plot the energy/time scaling parameter $\lambda(t)$ as a black curve enveloping the six energy ratios given in Eq. (10). A small $\lambda(t)$ speeds the quantum computer through times when the internuclear distance R is large, but as R decreases ($t \rightarrow 0$), a relatively small g_{max} value constrains the growing couplings. $\lambda(t)$ increases over two orders of magnitude, creating a highly nonlinear relationship between t_{qc} and t , as shown in Fig. 1(c). This effectively stretches the portion of the collision when internuclear distance is small over the entire simulation, as can be seen in the plot of the quantum computer's control parameters as a function of t_{qc} in Fig. 1(d).

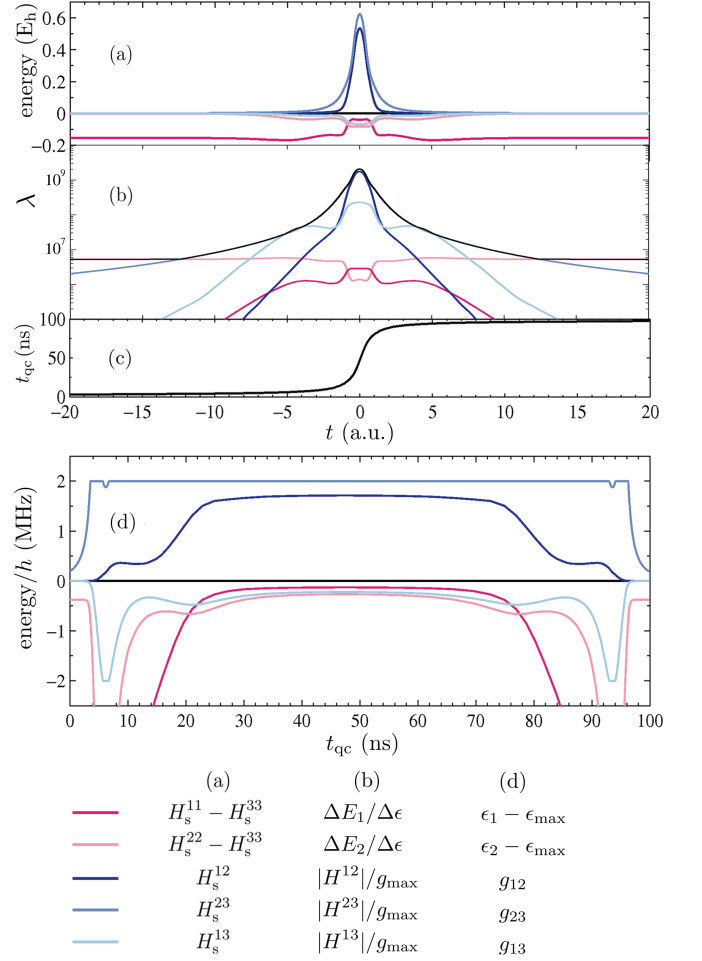


FIG. 1: (color online) $H_s(t)$ describes a three channel Na-He collision with $b = 0.5$ and $v = 1.0$. (a) Matrix elements of H_s as a function of time in atomic units ($E_h = 27.21 \text{ eV}$ and the atomic unit of time is $2.419 \times 10^{-8} \text{ ns}$). (b) The dimensionless time scaling parameter $\lambda(t)$ envelopes six energy ratios ($\Delta E_3 = 0$ for all t). We assume $g_{\text{max}}/h = 2.0 \text{ MHz}$ and $\Delta \epsilon_{\text{max}}/h = 190 \text{ MHz}$. (c) Plot of $t_{\text{qc}}(t)$ for the case of $t_{\text{qc}}(t_i) = 0$, $t_i = -40 \text{ a.u.}$. (d) Control parameters that simulate $H_s(t)$ plotted as a function of t_{qc} ($\epsilon_3 = \epsilon_{\text{max}}$ for all t_{qc}).

To study the fidelity of the simulation, we compare the exact and simulated time evolution operators, $U(t)$ and $U_n(t_{\text{qc}}(t))$ respectively, by plotting (in Fig. (2)) transition probabilities out of $|1\rangle$:

$$P_{1i}(t) \equiv |\langle i | U(t) | 1 \rangle|^2. \quad (16)$$

Because the exact transition probabilities evolve differently with t than the simulated evolve with t_{qc} , we define a time-dependent transition fidelity which accounts for time scaling,

$$F(t) \equiv |{}_s \langle 1 | U^\dagger(t) U_n(t_{\text{qc}}(t)) | 1 \rangle_n|^2, \quad (17)$$

and a time-dependent leakage out of \mathcal{H}_n ,

$$L(t) \equiv \sum_{\perp} |{}_s \langle i | U_{\text{qc}}(t_{\text{qc}}(t)) | 1 \rangle_n|^2 \quad (18)$$

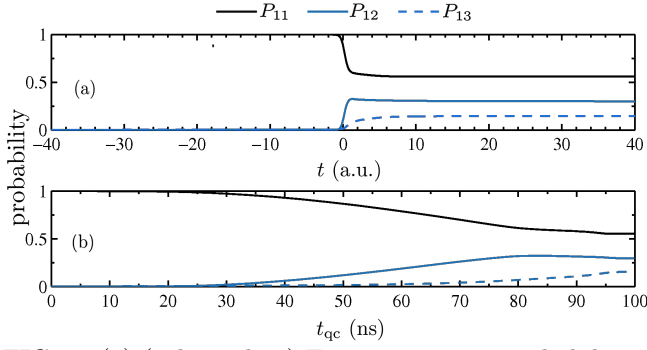


FIG. 2: (a) (color online) Exact transition probabilities generated by $H_s(t)$ shown in Fig. 1(a). (b) Transition probabilities simulated with parameter profiles given in Fig. 1(d). Final simulation fidelity is 0.998.

where \sum_{\perp} is the sum over all computational basis states $|i\rangle_{\perp}$ orthogonal to \mathcal{H}_n . In the upper part of Fig. (3), fidelity and leakage are plotted together for four different g_{\max} values.

Minimizing $g_{\max}||J_{\mu\nu}||/\epsilon_{\min}$, either by decreasing g_{\max} or by increasing ϵ_{\min} , reduces leakage and thus improves simulation fidelity. In this example, we find simulation fidelity more sensitive to the cutoff in g_{\max} because leakage is most prominent when the interatomic distances are small ($t \rightarrow 0$) and the diabatic couplings between channels are the dominant terms. By reducing g_{\max} we also increase $\lambda(t)$ and thus the total simulation time, as studied in the lower plot of Fig. (3). To increase fidelity from .9990 to .9999 we need to increase the simulation time by a factor of ~ 3 , a relationship that is independent of n . While not introducing specific models of decoherence, we note that high fidelity simulations are possible on superconducting qubits with coherence times around 100 ns.

When applied to molecular collisions, our approach to quantum simulation requires classical overhead to project the fundamental, time-independent, many-body Hamiltonian into an R -dependent, n -channel H_s . The quantities of physical interest, cross sections, are obtained by integrating the final transition probabilities over many semiclassical trajectories with different impact parameters, which requires no further classical overhead. A classical simulation of transition probabilities requires $\sim n^3$ elementary operations per time step for a single impact parameter, thus cross section calculations are computationally intensive for large n . Alternatively, simulation time is independent of n using our protocol, so once the R -dependent H_s has been calculated, cross sections can be obtained quickly.

In summary, we have presented a straightforward protocol for quantum simulation that can be implemented with currently available superconducting quantum computing technology. While a promising application of quantum computation, current quantum simulation protocols require a threshold number of gates and qubits

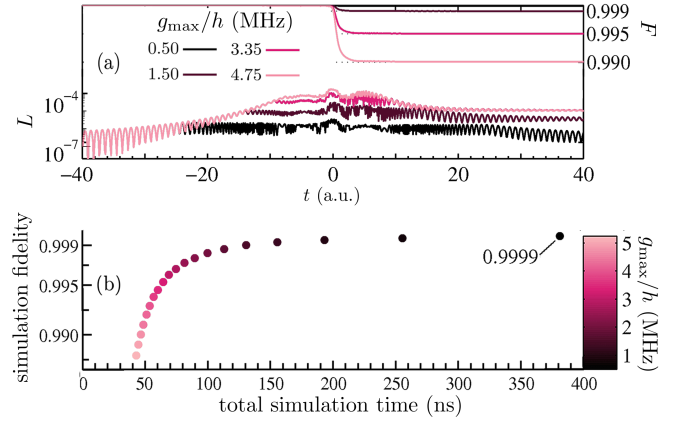


FIG. 3: (color online) (a) Fidelity and leakage as a function of simulation time for four different g_{\max} values, with all other parameters the same as in Fig. 1. (b) Final simulation fidelity versus total simulation time for varying g_{\max} . The g_{\max} value is referenced by the shade of the data point.

that prohibits fully digital quantum simulations from being demonstrated on available quantum computers. However, we have shown how quantum computers of only a few qubits can simulate arbitrary quantum systems accurately and quickly even before they reach the regime of fault tolerant quantum computation.

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